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RPPR Final Report
as of 27-Dec-2018

Agency Code:

Proposal Number: 72847CHCF **Agreement Number: W911NF-18-1-0112**
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DUNS Number: 078763334 EIN:
Report Date: 30-Nov-2018 Date Received: 21-Dec-2018
Final Report for Period Beginning 01-Mar-2018 and Ending 31-Aug-2018
Title: Financial Support for American Chemical Society Symposium for Ionic Liquids Research
Begin Performance Period: 01-Mar-2018 **End Performance Period:** 31-Aug-2018
Report Term: 0-Other

Submitted By: Scott Shaw Email: scott-k-shaw@uiowa.edu
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STEM Degrees: **STEM Participants:**

Major Goals: The purpose of the symposium was to bring together an international group of Ionic Liquid chemistry researchers at the 255th Meeting of the American Chemical Society, scheduled for the 18th to 22nd of March, 2018, in New Orleans, LA.

The primary objectives for this symposium are listed here:
1. To share state-of-the-art ionic liquids research, including collegial feedback, to strengthen academic rigor of the field
2. To create shared visions to employ ionic liquids in solutions to major societal challenges, i.e. energy storage and transformation
3. To facilitate collaborative research ideas across disciplines and geographic locations
4. To expand awareness of ionic liquids research, and bring new researchers into the field
5. To support the participation of new and young investigators in ionic liquid research

Topics to be covered:
The symposium was organized to contain six thematic topics including:
1. Computation and Theory of Ionic liquids
2. Ionic Liquid in Electrochemistry and Energy
3. Ionic Liquids Dynamics and Structure
4. Ionic Liquids at Surfaces and within Interfaces
5. Physical Properties and Applications of Ionic Liquids
6. Biomass Conversion using Ionic Liquids

The location and probable date(s) and why the conference was considered appropriate at the time specified:
The symposium coincided with the 255th ACS National Meeting, scheduled for 18-22 March, 2018, in New Orleans, Louisiana. This meeting regularly draws thousands of professional chemists form industry and academia. New Orleans is an attractive venue for domestic and international speakers. The Ionic Liquids symposium proposed here was co-listed by two divisions of the American Chemical Society; the Division of Physical Chemistry and the Division of Colloid and Surface Chemistry. This significantly broadened the pool of participants and attendees. A shortage of focused programing in the Ionic Liquids area had created an increased demand for this focused symposium, and it received an excellent rate of participation as described in the "Accomplished" section below.

An explanation of how the conference will relate to the research interests of the Army and how it will contribute to

the enhancement and improvement of scientific, engineering, and/or educational in general and activities as outlined earlier in the research areas of this BAA.
Ionic liquids (ILs) research is relevant to several areas of ARO interest including electrochemistry, catalysis, materials science, reaction dynamics, and interfacial activity. Research in these areas provides a framework of knowledge for nascent applications of ILs related to energy storage devices, ILs as fuels, ILs as solvents for biomass conversion, and ILs' role in separations chemistry. In each of these areas the combination of experiment and theory is required to elucidate properties and behaviours of ILs, both in the bulk phase and at the chemical interface. In particular, the nature of ionic liquid materials makes them intriguing solvents for electrochemistry, and recent studies have revealed several different naturally occurring size-domains that range from a few nanometers to several microns in dimension. The ramifications of these findings extend to the dynamics of IL systems, which have shown responses to applied electric potentials that defy long-standing electrochemical theories. This is particularly true of the IL-electrochemical double-layer structure and capacitance, which shows very slow dynamics which may directly affect heterogeneous catalysis, ionic transport through IL materials, and the development of ionicity models of IL solvents when mixed with molecular co-solvents (i.e., acetonitrile).

The name of chairperson(s)/(PI)(s) and his/her biographical information:
There were five co-chairs of this symposium, listed below:
Ed Castner, Rutgers University, ed.castner@rutgers.edu
Ed Maginn, University of Notre Dame, ed@nd.edu
Claudio Margulis, University of Iowa, claudio-margulis@uiowa.edu
Scott Shaw, University of Iowa, Scott-k-shaw@uiowa.edu
Jim Wishart, Brookhaven National Lab, wishart@bnl.gov

A list of proposed participants and the methods of announcement or invitation:
The symposium consisted of 65 oral presentations (invited and contributed talks) and 7 poster presentations spread over the five days of the ACS meeting. The symposium program is attached as a separate PDF file. The ACS meeting and Ionic Liquids symposium was broadly advertised to U.S. and International audiences via directed emails and advertising in major publications/magazines.

Budget:
Total project conference costs by major cost elements
The symposium costs included:
i. Travel to and from the Ernest N. Morial Convention Center in New Orleans
ii. Accommodation while at the symposium, typically arriving Saturday, 11th March and departing Thursday, 16th March, 2018
iii. Registration costs paid to the American Chemical Society which is hosting the symposium as part of their National Meeting. The American Chemical Society provides logistical support, the venue for the sessions of this symposium, and advertising for the symposium.

Sources of conference income and amount from each:
The total expected symposium budget was $10,000. $3000 of this came from ARO.
i. $3,000 from DOD-ARO
ii. $3,000 via a matching award mechanism from the American Chemical Society’s Division of Colloid and Surface Chemistry
iii. A set of amount of $400 per each filled am/pm symposium session provided by the American Chemical Society’s Division of Physical Chemistry. The symposium filled 9 oral sessions and contributed to 1 poster session, and received $4000.

Use of funds requested:
The entire symposium budget, including the $3,000 from ARO, was used to offset travel and accommodation expenses for invited speakers. Young investigators, who would otherwise not have funds to attend the meeting, were preferred recipients. Further details are given in the "Accomplished" section.

Accomplishments: The symposium was held as planned. The conference program is attached as a separate PDF file.

To support the objectives outlined in the "Major Goals" section, the organizers confirmed the participation of over 30 international leaders who lead productive research programs in several key areas of current ionic liquids research. The invited speakers each delivered a 30-minute presentation on the most recent and exciting ionic

liquids research produced by their groups. The invited speakers anchored the symposium and their presentations drew large numbers of participants/audience members. In addition to invited speakers an additional 30-40 contributed talks were accepted, as well as a similar number of poster presentations. The contributed talks were each of 20-minutes duration and provided an opportunity for many other researchers in IL areas to have their results featured among many leaders in the field. The symposium also offered several discussion-intermissions to allow small groups of participants and attendees to discuss results or questions in greater detail. Together with the poster presentations, this created a symposium series that spanned the entire five days of the ACS National Meeting.

The requested funds were used as planned. The additional support was received from the ACS Division of Physical Chemistry and Division of Colloid and Surface Chemistry. Awards were made in the range of $400 to $700 to speakers who were Young Investigators and requested financial assistance. The goal of the awards was to offset ca. 50% of the participant's total costs (travel + accommodation + registration) to attend the symposium. All of the reimbursements have been made.

Training Opportunities: This symposium presented the most recent research in the areas outlined above arising from new computational and experimental approaches. The presentations and discussions added to our understanding of IL systems' behaviors under variable electrochemical, thermal, pressure, and fluid flow conditions. The participants in this symposium gained a knowledge of these important aspects of ionic liquid chemistry, improving research productivity and effectiveness across the community.

Results Dissemination: A summary of how the results of the meeting will be disseminated:
Presentation titles and abstracts were disseminated online and in text by the ACS National Meeting. The symposium participants (registered speakers) were encouraged to share their presentations and data with each other and other attendees freely (to the extent possible) via digital file sharing. Any person who had registered for the ACS National Meeting was allowed to attend and participate in the discussions before/after all presentations.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Scott Shaw
Person Months Worked: 1.00
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

RPPR Final Report
as of 27-Dec-2018

255th American Chemical Society National Meeting & Exposition
New Orleans Convention Center, New Orleans, LA
March 18th – 22nd, 2018

Conference Proceedings for:

PHYSICAL CHEMISTRY OF IONIC LIQUIDS

Ernest N. Morial Convention Center, Room 214
Sponsored by the PHYS and COLL divisions
Financially Supported by US-ARO

SUNDAY MORNING

Physical Chemistry of Ionic Liquids: Functional Ionic Liquids & Applications

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

T. L. Greaves, *Presiding*

8:30 Introductory Remarks.

8:35 : 23. Chemistry and space propulsion applications of room-temperature ionic liquids. **S.D. Chambreau**, G.L. Vaghjiani, S. Schneider

8:55 : 22. Infrared spectroscopy studies of the hypergolic reaction and decomposition of a dicyanoborohydride ionic liquid. **A.E. Thomas**, S.D. Chambreau

9:15 : 24. Azole-functionalized boranes: Bringing the tunability of ionic liquids to molecular systems. **R.D. Rogers**

9:35 : 25. On the creation and chemistry of ionic liquids stable in air for months at 300ºC. **J.H. Davis**, K.N. West, B. Rabideau, T.G. Glover, B. Siu, R.A. O'Brien, M. Soltani, C. Cassity, M. Vo, J. McCants, E.A. Salter, A. Wierzbicki, A.C. Stenson, J.L. McGeehee

10:10 Intermission.

10:25 : 26. Porous ionic liquids: structures and dynamics. **S. Dai**

11:00: 27. Porous liquids from metal organic frameworks in ionic liquids. **M. Costa Gomes**, L. Pison, C. Cervinka, A. Padua

11:35 : 28. Solvent extraction in ionic liquids: Structuration and aggregation effects on extraction mechanisms. **S. Dourdain**, T. Sukhbaatar, G. Arrachart, S. Pellet-Rostaing

SUNDAY AFTERNOON

Physical Chemistry of Ionic Liquids: Functional Ionic Liquids & Applications

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

R. Hayes, *Presiding*

1:30: 63. Choline-Amino Acid Based Ionic Liquids – From Solvent Structure to Lignin Dissolution. **H. Jiang**, G. Warr, R. Atkin, S. Imberti

1:50: 64. Ionic liquids as catalysists for biomass conversion. **K. Takahashi**

2:25 : 65. Comparison of imidazolium- and cholinium-based ionic liquids for biomass pretreatment and "one-pot" conversion technologies. **B.A. Simmons**

3:00: 66. Pseudoprotic ionic liquids and protic mixtures: Strange cousins of ionic liquids. **M.N. Kobrak**

3:20 Intermission.

3:35 : 67. High throughput and machine learning approaches to characterising stoichiometric and non-stoichiometric protic ionic liquid-water solutions. D. Yalcin, C. Drummond, **T.L. Greaves**

4:10: 68. Ionic liquid electrolytes for harvesting low-grade waste heat. **J. Pringle**, M. Dupont, A. Taheri, D. Al-Masri, D.R. MacFarlane

4:45 : 69. A detailed study on thermophysical properties of natural deep eutectic solvents via combined experimental and theoretical approaches. S. Aparicio-Martinez, **M. Atilhan**

MONDAY MORNING

E. Castner, E. Maginn, C. J. Margulis, J. F. Wishart, *Organizers*

<officer>S. K. Shaw, *Organizer, Presiding*

8:30: 112. Electrode-ionic liquids interfaces: Determination of the potential of zero charge and characterization of slower charging processes. **N.M. Vargas-Barbosa**, B. Roling

8:50: 113. Solvation dynamics of an ionic and a molecular probe in an ionic liquid and an deep eutectic solvent with similar structure. Y. Cui, **D.G. Kuroda**

9:10: 114. Electrochemistry and electrochemical processing in deep eutectic solvents. **K.S. Ryder**, A.P. Abbott, A. Hillman

9:45 : 115. Tunable and stiff solid electrolyte made from an ionic liquid and a rigid-rod polyanion. **C. Zanelotti**, Y. Wang, S.E. Wollman, D. Yu, R. Kerr, M. Hegde, T.J. Dingemans, M. Forsyth, L.A. Madsen

10:05 Intermission.

10:20: 116. Magnetic control of ionic liquid ions in the electrical double layer. **R. Hayes**

10:55 : 117. Viscosity dependent dynamics of electrochemically driven molecular reorientations revealed via vibrational spectro-electrochemistry. **A. Horvath**

11:15 : 118. Directing bulk and interface interactions in ionic liquids to modulate ion solvation, conduction and structure in electrochemical systems. **B. Gurkan**, Q. Huang

11:35 : 119. Ion diffusion in ionic liquids in electric fields. R.A. Clark, J. Edel, B. Kirchner, M.K. Kuimova, A.J. McIntosh, M.A. Nawawi, M. von Domaros, **T. Welton**

MONDAY AFTERNOON

Physical Chemistry of Ionic Liquids: Electrochemistry and Electrochemical Interfaces

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

K. S. Ryder, *Presiding*

1:30: 165. Local electric fields at the interfaces of ionic liquids and metals measured by Stark shift spectroscopy. J. Patrow, **J. Dawlaty**

1:50: 166. Electrode reactons in ionic liquids. **D.V. Matyushov**

2:25 : 167. Statics and dynamics of crowding at an electrode–ionic liquid interface: X-ray scattering studies. M. Chu, M. Miller, T. Douglas, **P. Dutta**

3:00: 168. Ordered ionic liquid structure observed at terraced graphite interfaces by reflection high-energy electron diffraction. **D. Yang**, C. Wu, X. He

3:20 Intermission.

3:35 : 169. Nitrogen reduction to ammonia in ionic liquids. **D. MacFarlane**

4:10: 170. Quasi-elastic and inelastic neutron scattering studies of glass-forming ammonium-based ionic liquids at low temperatures. **T. Lima**, Z. Li, M.C. Ribeiro, Y. Zhang

4:30: 171. Ion structure and dynamics in highly concentrated ionic liquid-alkali metal salt electrolytes. **M. Forsyth**, P. Howlett, F. Chen, D. MacFarlane

TUESDAY MORNING

Physical Chemistry of Ionic Liquids: Computation, Theory & Simulation

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

S. Garrett-Roe, *Presiding*

8:30: 233. Large scale molecular simulations to interrogate nanostructuring and transport in transformational solvents for CO_2 capture. **V. Glezakou**, R. Rousseau, M. Nguyen, D.C. Cantu, D. Malhotra, D.J. Heldebrant, P. Koech, J. Page

8:50: 234. Role of quadrupolar interactions in the solvation of carbon dioxide in ionic liquids. **S. Corcelli**

9:25 : 235. Structure in conventional and not so conventional aromatic ionic liquids. **K. Shimizu**, J. Canongia Lopes

10:00: 236. Mesoscale structural and dynamic correlations in ionic liquids sampled by atomistic molecular dynamics simulations. **D. Bedrov**, D. Dong, M. Ebrahiminia, J. Vatamanu

10:20 Intermission.

10:35 : 237. What we learn from resolving dispersion and polarization interactions of ionic liquids. **A. Padua**

11:10: 238. Dynamical and dielectric properties of an ionic liquid using a charge transfer, polarizable model. **S.W. Rick**, C. Schroeder, A.S. Lyons

11:30: 239. Polarizability effects in ionic liquids. **C. Schröder**

WEDNESDAY MORNING

Physical Chemistry of Ionic Liquids: Structure

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

K. Shimizu, *Presiding*

8:30: 287. Implications of liquid structure on the vibrational spectra of ionic liquids. **C. Burba**

8:50: 288. Thermal and neutron scattering studies on alkylammonium-based ionic liquids with plastic-crystalline phases. **O. Yamamuro**, M. Nirei, M. Kofu, M. Matsuki, T. Yamada, T. Madhusudan

9:25 : 289. The Importance of Polarizability in the Solvation of Molecular Solutes in ionic liquids: OHD-RIKES measurements and molecular dynamics simulations on mixtures of CS_2 and ionic liquids. **E.L. Quitevis**, R.M. Lynden-Bell

10:00: 290. Spectroscopic and calorimetric analysis of multiple ionic liquid phase transitions in bulk and thin film systems. **J. Wrona**, S.K. Shaw

10:20 Intermission.

10:35 : 291. Mesoscopic structural organization in triphilic, fluorinated, room temperature ionic liquids. **O. Russina**

11:10: 292. Liquid structure and self-assembly in ternary ionic liquid systems. H. Jiang, R. Atkin, **G. Warr**

11:45 : 293. Elucidating the microscopic mechanics of attractive cation-cation interactions in hydroxyl-functionalized ionic liquids by isomer-selective vibrational spectroscopy of the N_2-tagged, gas phase $(M^+)_2NTf_2^-$ ternary complexes. **F. Menges**, **H. Zeng**, T. Niemann, A. Strate, R. Ludwig, M.A. Johnson

WEDNESDAY AFTERNOON

Physical Chemistry of Ionic Liquids: Transport & Dynamics

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

O. Russina, *Presiding*

1:30: 338. Simulations of friction on solute motion in ionic liquids. B. Conway, C.A. Rumble, **M. Maroncelli**

2:05 : 339. Ionic liquid mobility on different time scales as seen from polar, apolar and solute perspectives. **C.J. Margulis**, R.P. Daly, J.C. Araque

2:25 : 340. Influence of mesoscopic confinement on the dynamics of room temperature ionic liquids. **M.D. Fayer**

3:00: 341. Hydrogen bond dynamics in protic ionic liquids: Ultrafast vibrational spectroscopy of SCN-. **S. Garrett-Roe**

3:35 Intermission.

3:50: 342. Effects of mesoscopic domain structure on shear viscosity of ionic liquids. **T. Yamaguchi**

4:25 : 343. Molecular origin of enhanced proton conductivity in anhydrous ionic glasses. **Z. Wojnarowska**, L. Tajber, J. Knapik-Kowalczuk, M. Paluch

4:45 : 344. Influence of mesoscale organization on charge transport and dynamics in ionic liquids. **T. Cosby**, Z. Vicars, M. Heres, K. Tsunashima, J. Sangoro

THURSDAY MORNING

Physical Chemistry of Ionic Liquids: Interfaces & Ionic Liquid Nanoscience

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

K. Schroeder, *Presiding*

8:30: 619. Taking a close look at ionic liquid / support interfaces. **H.-P. Steinruck 9:05: 618.** Re-structuring of molten inorganic salts and ionic liquids around Nanoparticles: Stable colloidal solutions. **V. Kamysbayev**, V. Srivastava, D.V. Talapin

9:25 : 620. Ionic liquid structure in bulk and at interfaces. B. Wu, M. Zhao, M.S. Emerson, Y. Wang, **E. W. Castner**

9:45 : 621. Structure and screening behaviour of ionic liquids under nanoconfinement. **C.S. Perez Martinez**, S. Perkin

10:05 Intermission.

10:20: 622. Probing the structure of an ionic liquid interface by reactive atom scattering. E.J. Smoll, S. Purcell, L. D'Andrea, J.M. Slattery, D.W. Bruce, M.L. Costen, K.G. McKendrick, **T.K. Minton**

0:40: 623. Following reactions in ionic liquids through the outer surface by X-ray photoelectron spectroscopy. **F. Maier**, H. Steinrueck

11:15 : 624. Effect of the environmental humidity on the interfacial properties of Ionic liquids. **R.M. Espinosa-Marzal**

11:50: 625. Reversible, micron-scale ordering in ionic liquid films. **R.S. Anaredy**, R. Specht, S.K. Shaw

THURSDAY AFTERNOON

Physical Chemistry of Ionic Liquids: Ionic Liquid-Solute-Solvent Interactions

E. Castner, E. Maginn, C. J. Margulis, S. K. Shaw, J. F. Wishart, *Organizers*

F. Maier, *Presiding*

1:30: 655. First principles molecular dynamics study of a deep eutectic solvent: Choline chloride/urea and its mixture with water. E.O. Fetisov, D.B. Harwood, I.W. Kuo, S.E. Warrag, M.C. Kroon, C.J. Peters, **J.I. Siepmann**

1:50: 656. Ionic liquid nanostructure enables alcohol self assembly. **R. Atkin**, T. Murphy, R. Hayes, S. Imberti, G. Warr

2:25 : 657. From cnidaria to mollusca: Bulk and surface structuration in ionic liquids. **J. Canongia Lopes**, K. Shimizu, A.A. Freitas

3:00: 658. Intermolecular interactions and vibrational perturbations in 1-ethyl-3-methylimidazolium thiocyanate/water mixtures. C.R. Hutchison, S.N. Johnson, C. Williams, N. Hammer, C.L. Hussey, **G.S. Tschumper**

3:20 Intermission.

3:35 : 659. Surface-active ionic liquids in water: Targeted nanoreactors for synthesis, catalysis and materials preparation. **K. Schroeder**, A. Cognigni, M. Hejazifar, R. Zirbs, C. Schröder

4:10: 660. Structural organization in protic ionic liquid/molecular liquid mixtures. **A. Triolo**, O. Russina

4:30: 661. Impact of alcohol size and identity on the dynamics of an imidazolium-based ionic liquid. **T. Miller**, S. Corcelli

4:50: 662. Effect of gas impurities on the CO_2 uptake in superbase ionic liquids. **R. Taylor**, H. Daly, A. Greer, J. Jacquemin, C. Hardacre

5:10 Concluding Remarks.